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Powder Diffraction Studies of the Ferrocene@ $[\text{Al}(\text{OH})(\text{bdc})]_x$ and Ferrocene@ $[\text{VO}(\text{bdc})]_x$. Kirill Yusenko^a, Mikhail Meilikhov^a, Roland A. Fischer^a. ^a*Inorganic Chemistry II - Organometallic and Materials, Ruhr-University Bochum, Germany.*
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The Coordination Polymers (CPs) with permanent porosity and high thermal stability are a unique class of hybrid solid-state materials with bright future [1]. The use of these materials ranges from gas storage, separation and catalysis, to a number of diverse potential applications, including optoelectronics, sensors, smart membranes etc. Also aiming at applications in catalysis we have introduced the solvent-free gas-phase loading of porous CPs via the adsorption of volatile organometallic all-hydrocarbon precursors [2]. We selected MIL-53(Al), $[\text{Al}(\text{OH})(\text{bdc})]$, and MIL-47(V), $[\text{VO}(\text{bdc})]$, as members of a huge family of porous CPs based on chains of *trans*-corner sharing octahedral units $\{\text{MO}_6\}$ cross-linked by bdc (terephthalic acid) which results in a 3D structure exhibiting 1D channels along the *a* axis. We were able to obtain the absorbate structures for ferrocene [3], ferrocenealdehyd, 1,1'-ferrocenedialdehyd, 1,1'-dimethylferrocene and 1,1'-diethylferrocene inside MIL-53(Al) and MIL-47(V) based on home powder X-ray diffraction (D8-Advance Bruker AXS diffractometer, Debye-Scherrer geometry) as a model compounds for the further applications. All data were indexed in the *Imma* and *Imm2* space groups. Positions of the guest molecules were obtained by global optimisation using the FOX software [4] starting from rigid "empty" MIL-53(Al) framework and guest molecules as building blocks. Finally, the model obtained was refined by the Rietveld method with Jana2000 software [5]. Our attention here was concentrated on the structure solution strategy, packing of the guest's molecules inside the 1D channels of the host structure; also structural effects of the substitute group in the guest molecule, guest-guest and host-guest interactions were investigated.

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Synthesis and Crystal structure of $[\text{BaCu}(\text{H}_2\text{O})_4(\text{OOC}-\text{C}_6\text{H}_4-\text{COOH})_2]_n$. Fadila Balegroune^a, Aouaouche Benkanoun^a, Achoura Guehria-Laidoudi^a, Slimane Dahaoui^b, Claude Lecomte^b. ^a*Laboratoire de Cristallographie-Thermodynamique, Faculté de Chimie, USTHB, BP32,*

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Recently, research on the synthesis and characterization of coordination polymers is greatly motivated by substantial interest in their fascinating structures with potential applications [1-2].

We selected 1,2-benzenedicarboxylic acid (H_2BDC) as a bifunctional ligand taking into account its multiple coordination sites that may generate structures of higher dimensions. The heterobimetallic title complex has been synthesized from aqueous solution of a mixture of H_2BDC acid, barium hydroxyde and copper nitrate. The structure has been reported previously[3], but the positions of the H atoms have not been determined. It has now been refined with new intensity data to significantly higher precision and with all H atoms. Moreover, the compound has been reported as a diaqua, dihydrate complex. Our study shows only coordination water molecules.

The asymmetric unit consists of one Ba(II) cation, one Cu(II) cation, two *o*-phthalate dianions and four coordination water molecules.

The two independent $[\text{BDC}]^{2-}$ ligands adopt different coordination mode. One ligand coordinates to four metal centers with $\mu_3-\eta^2-\eta^1$ and $\mu_2-\eta^2$ -bridging coordination modes. The second ligand is linked to three metal centers with $\mu_2-\eta^1-\eta^1$ and $\mu_2-\eta^2$ -bridging coordination modes respectively. The Cu(II) cation presents a distorted square pyramidal coordination, which involves a CuO_4 equatorial plane containing three oxygen phthalate and one oxygen water atom. The axial position is occupied by a coordinated water molecule with a long Cu–O length of 2.277(3) Å due to the Jahn–Teller effect of Cu(II) ion.

The coordination geometry around the Ba(II) can be best described as a distorted tricapped trigonal prism. Among all the nine coordinated oxygen atoms, three come from coordinated water molecules and the remaining from five $[\text{BDC}]^{2-}$ dianions ligands. The BaO_9 polyhedra share faces to form zigzag chains running along the [010] direction via water bridges, and linking *o*-phthalate atoms. This results in Ba...Ba separations of 4.210(1) Å. Consequently, the two-dimensional polymeric structure of the title compound consists of BaO_9 chains and CuO_5 polyhedra linked together through asymmetric *o*-phthalate bridges, the Ba...Cu distances being 4.340(1) and 6.298(1) Å respectively.

There is extensive hydrogen bonding in the structure, involving all the coordinated water molecules and the O atoms of the carboxylate groups.

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